# QSAR model for skin permeability (v1.0)

ProtoADME by ProtoQSAR

## ProtoADME

ProtoADME is a computational (*in silico*) tool focused on the prediction of endpoints related with the ADME (Absortion, Distribution, Metabolism and Excretion) of chemical substances.

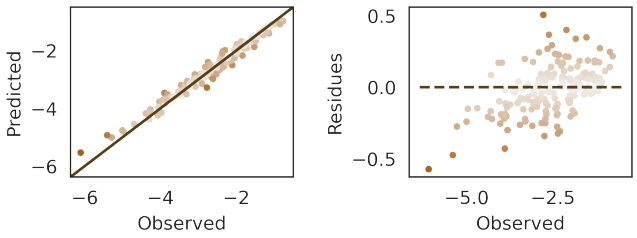
## Endpoint

**Toxicokinetic: skin permeability**

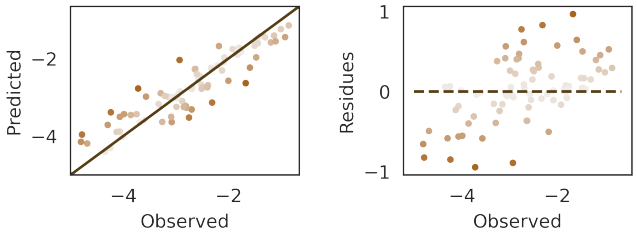
Skin permeability is a measure of the absorption of a compound through the outer surface of the skin.

## Metrics

### Training set




### Validation set




| Parameters | Training | Validation |
|---|---|---|
| $R^2$ score | 0.97 | 0.84 |
| Mean absolute error (MAE) | 0.13 | 0.30 |
| Mean squared error (MSE) | 0.03 | 0.16 |
| Median absolute error | 0.09 | 0.24 |
| Explained variance | 0.97 | 0.84 |

ProtoADME is part of ProtoPRED

ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, by proprietary (Q)SAR models.

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